DESIGN OF ALUMINUM ALLOY FOR SIMULTANEOUS ENHANCEMENT OF STRENGTH AND ELECTRICAL CONDUCTIVITY USING MACHINE LEARNING

Dissertation submitted to
Visvesvaraya National Institute of Technology, Nagpur
in partial fulfillment of the requirements for the award of
the degree

Master of Technology
in
Process Metallurgy

by

Vaibhav Paigwar

MT23PME001

under the guidance of

Dr. Rajesh Khatirkar

Department of Metallurgical & Materials Engineering
Visvesvaraya National Institute of Technology
Nagpur 440010 (India)
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Declaration

I, hereby declare that the dissertation titled **"Design of Aluminum alloy for Simultaneous Enhancement of Strength and Electrical Conductivity using Machine Learning**" submitted herein has been carried out by me in the Metallurgical and Materials Engineering of Visvesvaraya National Institute of Technology, Nagpur. The work is original and has not been submitted earlier as a whole or in part for the award of any degree/diploma at this or any other Institution/University.

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Date:

Certificate

This is to certify that the dissertation titled **"Design of Aluminum alloy for Simultaneous Enhancement of Strength and Electrical Conductivity using Machine Learning"** is submitted by **Vaibhav Paigwar** in partial fulfillment of the requirements for the award of the degree of Master of Technology in Process Metallurgy, VNIT, Nagpur. The work is comprehensive, complete and fit for final evaluation.

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Vaibhav Paigwar

ABSTRACT

This work presents a machine learning-based aluminum alloy design approach. Machine learning accelerates the prediction and optimization of alloy compositions and desired attributes, decreasing the entire material development cycle. The main objective of the work presented in this thesis is the design of an Al alloy that has good value for both ultimate tensile strength (UTS), and electrical conductivity (EC). Aluminum alloys that are strong often lose conductivity due to solute atoms (substitutional as well as interstitial) and precipitates (second phase particles) that scatter electrons. Conversely, pure aluminum has excellent conductivity but poor strength. Achieving both properties is a challenging task and requires careful alloy design. Such alloys have applications in overhead power transmission lines, electric vehicle (EV) battery, busbars, aerospace wiring, railway electrification, etc. To address this design task machine learning (ML) models are utilized. The prediction of alloy compositions is an inverse design problem. A total of eight machine learning algorithms were trained to first predict the desired mechanical property using the element compositions. Among these models, Gradient Boosting Regression (GBR) algorithm was found to be the best performing model. This model was then used to find the important alloying elements for training the forward regressor. For the inverse prediction, optimization approach is utilized by using Genetic algorithm with GBR. Different aluminum alloys exhibiting high values for properties-UTS and EC have been presented. The predicted alloy compositions for a desired mechanical property value are verified using the forward gradient boosting regressor. Experimentation on multi-objective model show that alloy with conflicting properties-UTS and EC can be designed using ML approaches. Further, experimental validation is done by casting three alloy compositions. For validation of individual UTS model, Al-Si alloy, and A643 alloy were cast. For simultaneous enhancement of UTS and EC A646 alloy was cast. It is observed that the predicted value and obtained mechanical property by physical experimentation were close. Proving the efficiency of leveraging machine learning for alloy design.

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Chapter 1

INTRODUCTION

1.1 Background

Alloys are designed to enhance the mechanical, corrosion, wear and other properties to meet specific performance requirements for a particular application. Metallurgists can produce materials with desirable properties, such as improved strength, enhanced resistance to corrosion, higher hardness, or enhanced thermal stability, by changing the elemental composition and thermo-mechanical processing. This is especially crucial for sectors where materials must function in harsh environments, such as aerospace, automotive, construction, and energy. While alloy designing, a desired behavior can be achieved by combining the appropriate alloying elements. Finding appropriate alloying elements using traditional materials design methodologies is time-consuming. Due to the enormous design space, these solutions become progressively difficult.

In order to expedite alloy development, an increasing number of integrated multi-scale multi-physics models have emerged [1]. The physics-based models frequently rely on the microstructure to relate composition values to attributes, yet the majority of the microstructures data is intangible. As a result, physics-based models frequently include assumptions that might create uncertainties and mistakes and induce error propagation. Machine learning (ML) is a potential tool that alleviate the issues in the integrated multi scale multi-physics models. Supervised ML models use existing experimental data to discover statistical patterns, which are used to forecast patterns for newly available and unseen data. Machine learning models have lately been applied to solve many material science challenges, and has received a lot of interest in the field of alloy design [2, 3]. ML can facilitate in prediction of various mechanical characteristics for unseen alloy compositions [4, 5], and prediction of alloys composition for a desired mechanical characteristics [6].

ML expedites the discovery of new materials by reducing the experimentation time and expenses necessary for traditional trial-and-error approaches [7, 8]. It utilizes existing databases, published literature, advanced data extraction algorithms, and

computational methodologies for design of effective alloys. By considering specific requirements and constraints, ML algorithms can recommend appropriate material composition, simplifying the design of performance specific alloys in metallurgy.

The present work focuses on design of aluminum alloy for enhanced ultimate tensile strength (UTS) and electrical conductivity (EC) using ML approach. Aluminum alloy design is particularly important since aluminum is widely used in various industries. The highest tensile stress a material can sustain before failing under tension is known as its UTS. The ability of a material to conduct electric current is referred to as EC. UTS and EC are inversely proportional and achieving a balance between these is challenging. High EC and UTS aluminum alloys are essential for applications needing both effective electrical performance and mechanical durability. The usage of such alloys could be very advantageous for power transmission lines, electrical cables, busbars, lightweight wire systems in aero-planes, electric vehicles, and high-performance cars.

1.2 Objectives

The main objectives of the present work are:

- Development of a ML model for prediction of alloy composition for desired values of UTS and EC (individually).
- Development of a multi-objective ML model for simultaneous enhancement of UTS and EC.
- Validation of the results by actual lab experimentation (casting, rolling, heat treatment etc.).

1.3 Key Contributions

The major contributions of the work presented in the thesis are listed below:

- Experimenting with various ML algorithms to find model for aluminum alloy design.
- Selection of most important features (alloying elements) for training the machine learning model.
- Prediction of alloy composition using inverse method for desired mechanical property values. Different alloys exhibiting high values for various properties like

- UTS, and EC were found using the gradient boosting regressor and Genetic Algorithm as optimizer for inverse prediction.

- Prediction of alloy composition using inverse method simultaneously enhancing the values of UTS and EC.
- Verification of the predicted alloy compositions using forward model.
- Experimental validation of the predicted alloy compositions by casting of alloys and measurement of properties.

1.4 Organization of Report

The report comprises of five chapters and is organized as follows. A review of the existing work for prediction of alloy compositions using machine learning algorithms along with various machine learning algorithms are presented in Chapter 2. Chapter 3 discusses the methodology. The results are presented in Chapter 4. Chapter 5 concludes the work with an assessment of the limitations of our methodology, a consideration of certain outstanding issues, and an examination of the future scope of work.

Chapter 2

LITERATURE REVIEW

The need for a new aluminum alloy with both high ultimate tensile strength (UTS) and high electrical conductivity (EC) is driven by modern engineering challenges, especially in sectors where light weight, mechanical performance, and electrical efficiency must all coexist. Electric vehicles (EVs) and aerospace industry require strong yet lightweight materials that also conduct electricity well for busbars, battery enclosures, structural-electrical hybrids. Traditional high-strength alloys like 7xxx series are too poor in EC, while high-EC alloys like 1xxx are too weak. In power transmission and distribution, aluminum is used in overhead conductors and cables where strength and conductivity are both important e.g., in windy regions or long spans. It also has application in electronics packaging. Heat sinks, housings, and conductors need moderate-to-high strength to survive mechanical stress, and high EC to minimize power loss. The characteristics and behavior of aluminum alloys are discussed below followed by discussion on alloy design using ML and various ML algorithms.

2.1 Metallurgical Characteristics and Mechanical Behavior of Aluminum Alloys

The aluminum alloys are categorized according to the alloying elements into different series. Each series has its specific applications, and these alloying elements provide the alloy various metallurgical properties. The following is the classification [9]:

- **1xxx series:** 1000 series are basically pure aluminum, having a minimum weight content of 99% aluminum. They can be work-hardened and are utilized in the food and packaging, chemical, and transformer industries.
- **2xxx series:** 2000 series are alloyed with copper. Steel-like strengths can be achieved by precipitation hardening in these alloys. Duralumin, which is aluminum alloyed with copper, was once the most widely used aerospace alloy. However, it was prone to stress corrosion cracking, and new designs are increasingly using the 7000 series. Due to the high strength and corrosion

resistance, many specifications of the 2000 series are generally used in the automotive, high-speed rail and aerospace components.

- **3xxx series**: 3000 series are alloyed with manganese, and can be work hardened. They are typically utilized in the construction and packaging sectors; examples include partition houses, mobile homes, cans, and containers for storing chemicals.
- **4xxx series:** 4000 series are alloyed with silicon. Variations of aluminium–silicon alloys are intended for casting (and therefore not included in 4000 series) are also known as Silumin.
- **5xxx series:** Because of their exceptional corrosion resistance and magnesium alloying, the 5000 series is appropriate for use in maritime applications. Out of all the non-heat-treated alloys, 5083 has the highest strength. Ships, vessels, pressure vessels, marine pipelines, airplane skeletons, and other similar structures are the primary applications where 5000 series is used.
- **6xxx series**: 6000 series are alloyed with magnesium and silicon. They can be precipitation hardened, machined easily, and welded, but not to the high strengths that 2000 and 7000 can achieve. One of the most often used general-purpose aluminum alloys is 6061.Custom extrusion molding can be used to create six series. Aluminum extrusion profiles are essentially what the 6000 series products are. These include profiles for doors and windows, kitchen and wardrobe cabinets, extruded aluminum heat sinks, aluminum tile, floor, and carpet edge trim, profiles for LED strip lighting, slotted aluminum extrusion, and more.
- **7xxx series:** The highest strengths of any aluminum alloy can be obtained by precipitation hardening the 7000 series, which are alloyed with zinc. The aerospace industry mostly uses aluminum alloys from the 7 series for aircraft frames, sheet components, screws, wings, etc.
- **8xxx series:** 8000 series are alloyed with other elements which are not covered by other series. Aluminium–lithium alloys are an example.

Different series of alloy have different mechanical properties. Pure aluminum has high electrical conductivity (~60% IACS) but low tensile strength (~90 MPa). Alloying increases UTS (can exceed 500 MPa), but typically decreases EC. Alloying elements introduce lattice distortions and these distortions scatter electrons, reducing conductivity.

Precipitation hardening (e.g., in 2xxx or 7xxx series) enhances strength but significantly reduces EC. Table 2.1 shows range of UTS and EC for different series.

Table 2.1. Range of UTS and EC for different aluminium alloy series

Alloy Series	Major Alloying element	UTS (MPa)	EC (% IACS)
1xxx	Pure Al	60-110	59–65
2xxx	Cu	200-550	30-40
3xxx	Mn	110-290	40-50
4xxx	Si	150-300	40-50
5xxx	Mg	200-350	30-40
6xxx	Mg-Si	200-350	40-55
7xxx	Zn	300-700	25-35
8xxx	Miscellaneous (Li, Fe, etc.)	100-300	20–60

2.1.1 Effects of alloying elements

Alloying elements significantly affect the properties of aluminum, enhancing its mechanical strength, corrosion resistance, machinability, and other characteristics depending on the application. An outline of the most popular alloying elements for aluminum and their effects is presented in Table 2.2. Elements like copper improve strength but reduce corrosion resistance. Magnesium improves both, but alloys with high zinc and copper content can be harder to weld. Adding silicon or iron can make alloys harder but less ductile.

2.1.2 Effect of deformation on electrical conductivity

Cold Rolling (room temperature rolling) increases dislocation density and internal stress in aluminum. Dislocations and defects scatter free electrons, which lowers EC. Hot rolling deforms metal at high temperatures, usually higher than the recrystallization temperature. There is minimal effect of hot rolling on EC. There is some dislocation development, but rolling reduces their negative impact on EC by causing dynamic recovery and recrystallization. After deformation, annealing promotes dislocation reduction, grain growth, and recrystallization. Dislocations are eliminated or rearranged, and internal lattice distortions are decreased. EC rises as a result of all these factors. Hot rolling and annealing are therefore recommended.

Table 2.2. Effect of most popular alloying elements on Aluminum

Element	Effect on Aluminum
Copper (Cu)	Increases strength and hardness; reduces corrosion resistance. Often used in aircraft alloys (e.g., 2xxx series).
Magnesium (Mg)	Increases strength and workability; good corrosion resistance. Common in 5xxx series (marine applications).
Manganese (Mn)	Improves strength and corrosion resistance; also improves ductility. Found in 3xxx series.
Silicon (Si)	Reduces melting point, improves wear resistance; often used in casting alloys (e.g., 4xxx series).
Zinc (Zn)	Significantly increases strength; often used with magnesium in high-strength 7xxx series (aerospace). May reduce corrosion resistance.
Iron (Fe)	Usually an impurity, but in controlled amounts it improves strength and wear resistance. Can reduce ductility.
Nickel (Ni)	Enhances strength at elevated temperatures and improves corrosion resistance.
Chromium (Cr)	Increases corrosion resistance and improves strength through grain structure control.
Titanium (Ti)	Acts as a grain refiner during casting, improving mechanical properties and uniformity.
Lithium (Li)	Reduces density and increases stiffness, often used in aerospace-grade aluminum-lithium alloys.

2.1.3 Microstructure of 7075

7075 alloy comprises of Zinc (5.6–6.1%) as primary alloying element. It also Magnesium (2.1–2.5%), Copper (1.2–1.6%), and other elements like Fe, Si, Cr, Mn, Ti in small amounts.

1. α-Al Matrix

- The primary aluminum phase.
- Forms the continuous background structure.

2. Intermetallic Phases

- $MgZn_2$ (η phase): Principal strengthening phase.
- Al_2CuMg (S phase) and Al_7Cu_2Fe, AlFeMnSi: May form at grain boundaries or interdendritic regions in as-cast alloys.
- Cr-rich dispersoids ($Al_{12}Mg_2Cr$): Help control grain structure.

3. Grain Boundaries

- These contain coarse precipitates or constituent particles, especially if not homogenized.

- These can also be sites for intergranular corrosion if overaged or improperly heat-treated.

2.1.4 Stress strain of different alloying elements

Stress and strain are fundamental concepts in materials science that describe how a material deforms under load. Stress is the force per unit area within a material. Strain is the deformation (elongation or compression) per unit length. A stress-strain curve combines a lot of information about the material and its behavior [10]. Information from stress-strain behavior of aluminum when alloyed with different elements is presented in table 2.3. It describes how each alloying element alters the mechanical response, particularly UTS, Yield Strength, and Ductility, which is usually reflected in the shape of the stress-strain curve. Based on this the characteristics of different series are as follows. 1xxx series are very ductile, low strength, 2xxx and 7xxx exhibit high strength and lower ductility, 5xxx and 6xxx have balanced strength and ductility. 4xxx series are more brittle, and have shorter strain range.

Table 2.3. Effect on Stress-Strain for different alloying elements

Alloying Element	Effect on Stress-Strain Curve
Copper (Cu)	- Higher yield strength and UTS - Lower ductility (more brittle)
Magnesium (Mg)	- Increased strength with good ductility - Moderate work hardening rate
Zinc (Zn)	- Significant strength increase (especially with Mg) - Ductility may drop
Silicon (Si)	- Strength increases slightly - Good wear resistance but not huge ductility changes
Manganese (Mn)	- Slightly higher strength - Maintains good ductility
Iron (Fe)	- Acts as an impurity - Increases strength a little - Reduces ductility sharply
Nickel (Ni)	- Increases high-temperature strength - Little effect on room temperature stress-strain behavior
Chromium (Cr)	- Improves strength and corrosion resistance - Minimal effect on ductility

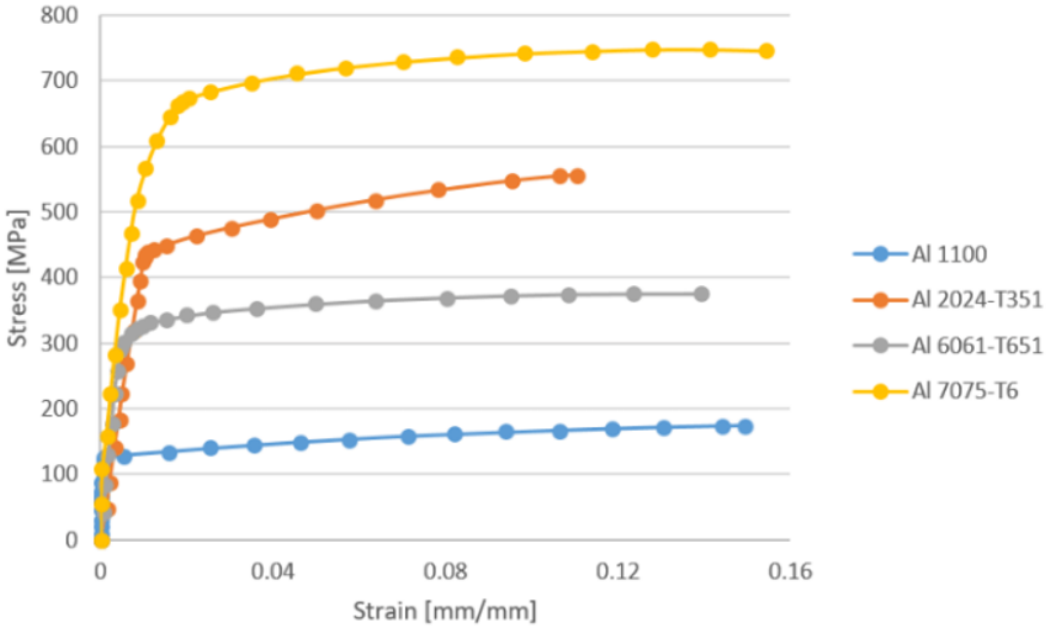


Figure 2.1. Stress-strain curve of different Al alloys (taken from [11])

2.2 Machine Learning and Alloy Design

In the recent years, ML has revolutionized the material science. It is common to automate research by using machine-learned models. ML models can predict the properties of new or untested alloy compositions based on existing data, allowing researchers to explore a vast space of potential materials efficiently. The ML model works by different model design strategies forward model design and inverse model design. Data-driven approaches have shown promising outcomes in inferring targets of interest (e.g. mechanical properties) from alloy features (elemental compositions). This process is known as forward model design. ML algorithm is trained using element composition values as features and target as property.

A further step in alloy design is the inverse design method, wherein suitable compositions and/or processing techniques are recommended based on specified performance requirements. This is the ultimate objective of material science and may substantially lower the time and expense involved in alloy design. The goal of inverse design is to discover alloy elements that have the specified property value. In [12], UTS and EC of copper alloy were taken as inputs, and 15 element compositions as outputs, a ML model is constructed to derive the composition of copper alloy based on target property.

2.2.1 Alloy Design using Inverse Method

Various machine learning algorithms used in the literature for alloy design are linear regression algorithm [13], non-linear regression ML algorithms such as k-nearest neighbour [14], support vector machine (SVM) [15], decision tree-based algorithms [16], Random Forests [17], ensemble algorithms [18, 19, 20] and Neural Networks [21]. In order to do regression analysis, linear regression algorithms attempt to fit a linear model. SVM determines the ideal hyperplane based on the largest possible margin. By splitting the dataset, the Decision Tree method creates a binary tree structure. To increase accuracy, Random Forest employs numerous decision trees. In order to recognize patterns and carry out predictive analysis, neural networks imitate the structure of the human brain. Further, these machine learning algorithms are used in conjunction with optimization algorithms such as Bayesian optimization, genetic algorithm, etc. to perform the inverse prediction.

In [22], many SVM models were trained, and the best-performing model was combined with a genetic algorithm as an optimizer to produce steel alloy. The results were validated by production. The results demonstrate the efficiency of the GA approach paired with the predictive model in the design of new alloys. A GA-driven inverse design using SVM, random forest, and XG Boost algorithms to design multicomponent-Ti alloys with a low Youngs modulus was used in [23]. In [24], a Support Vector Regressor model (SVR) with the radial basis function as the kernel function is used to predict the composition for Cu alloys having high UTS and EC. They have 27 samples of alloys. SVM along with Bayesian optimizer is used in [2], to obtain precipitation strengthened copper alloys. A method for creating aluminum-lithium (Al-Li) alloys with a high particular modulus and specific strength utilizing SVR was presented by Li et al. [25]. The authors compared the model predictions with experimental data from the literature and employed 10-fold cross-validation to validate the SVR models. ANN and SVM are used in [26] to describe the mapping between features and mechanical properties of magnesium alloy. The yield strength, ultimate tensile strength, and tensile elongation parameters were accurately predicted by the ML models.

Similar ML algorithms have also been used to develop the compositions of piezo electric materials [27] and inorganic superconductors [28]. In addition to simple alloy design, ML is also used for High-entropy alloys (HEAs). Various ML models with genetic algorithm are used in [29]. Apart from ML algorithms, neural networks are also

utilized in the literature. In [30], the ANN algorithm was adopted to correlate the composition and processing parameters of interstitial free (IF) steel sheets to their corresponding mechanical properties. For elongation and UTS, respectively, two ANN models were trained and adjusted. Following that, these models were applied as a fitness function for every characteristic independently. A Pareto frontier maximizing both elongation and UTS was built by an iterative evolution of the IF steel alloys. The collection of non-dominated solutions that resulted produced IF steels with various strength and ductility combinations.

2.2.2 Multi-Objective Alloy Design

Alloy design with only one objective mechanical properties are well addressed by machine learning. Improving multiple properties at the same time, on the other hand, is challenging.

Artificial neural networks (ANNs) and deep neural networks (DNNs) have been used in recent years to address Al alloy design with contradictory characteristics. Aluminum alloy with ultra-strength and high-toughness is presented in [31]. The toughness K_{IC}=33.9 MPa·m$^{1/2}$ and strength of 736 MPa was obtained. To train the ANN, a dataset of 171 alloy compositions from the literature that included high-strength and high-toughness aluminium alloys is used. In [32], a Bayesian optimization-based algorithm was utilized to obtain an alloy with high yield strength and Enlongation. With an elongation (EL) of 19% and a yield strength (YS) of 712 MPa, the new Al alloy offers a great balance of strength and ductility. To suggest novel chemical compositions and fabrication processes, a DNN model is utilized. However, less data in 100s or even thousands is a challenge for ANNs and lead to reduced performance. The availability of authentic data is very less for alloys, thereby making use of ANNs less beneficial.

Thereby, in the present work the possibility of using traditional ML methods, considering less data availability is explored. A feasibility study of machine learning-assisted alloy design using wrought aluminum alloys as an example is presented in [33]. The experimentations are performed with only composition- properties dataset of size 200 alloys, and properties like UTS, TYS, El, BHN, shear, and endurance. For each property there are at least 100 alloy values. Experimentation with SVM, Random Forest Algorithm and XGBoost shows ML models can work well even with low data. ANN

performs poor due to lack of data. The inference is that for less data use ML algorithms with proper hyper-parameter tuning gives better performance. As a result, the proposed work uses a machine learning approach rather than ANNs.

Feng et al. [34] combined a random forest model with the Non-dominated Sorting Genetic Algorithm (NSGA-II) to optimise strength and ductility. As a result, an Aluminum alloy with a tensile strength of 410 MPa and an elongation of 15.2% was successfully predicted. A prediction model for Aluminum alloy design with both high strength and thermal conductivity (TC) is presented in [8]. It makes use of support vector machine (SVM) and eXtreme gradient boosting (XGBoost) approaches. Alloy with TC over 190 $W \cdot m^{-1} \cdot K^{-1}$ and UTS over 220 MPa is predicted.

In the literature there no effort has been made to create an aluminum alloy with high EC and UTS. Copper based alloys for UTS and EC are a bit explored. For instance, a copper alloy with high UTS and EC is presented in [35]. They utilized 27 alloys with 69 Features. They used 69 features in 27 alloys. The important features found by correlation screening, recursive elimination and exhaustive screening are subjected to the Random Forest machine learning technique. The found alloys had UTS and EC values between 262 MPa and 298 MPa and between 68.5% and 90.4% IACS.

2.3 Machine Learning Algorithms

The Inverse models require predicting the element composition using mechanical property, that is, the target is to obtain a numeric value as the prediction using numeric values, thereby, regression models are used. The output of any regression model has a continuous value. In other words, a multivariate function with continuous values is calculated using the regression model. In this section, the most popular regression models used in this work are discussed.

2.3.1 Linear Regression

Linear regression (LR) [13] is a ML approach that models the relationship between the features (independent variables) and the target (dependent) variable. If there is one feature and one target variable then it is called as simple LR. The best- fitting straight line that minimizes the variation between the predicted and actual values is found using simple linear regression. If there are more than one features and one target variable then

it is called as multiple linear regression. The fundamental concept is to identify the best fitting hyperplane that reduces the difference between the dependent variables actual and predicted values.

2.3.2 Support Vector Regression

Support Vector Regression (SVR) [15] is a ML approach that tries to reduce the prediction error, or the difference between the intended and the predicted results. For set of features $X=\{x_1,x_2,\ldots,x_n\}$ and target values $Y=\{y_1,y_2,\ldots y_n\}$, SVR minimizes the objective function expressed in equation below,

$$\text{Minimize: } \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i^*)$$

Subject to:

$$y_i - (w^T\phi(x_i) + b) \leq \epsilon + \xi_i$$

$$(w^T\phi(x_i) + b) - y_i \leq \epsilon + \xi_i^*$$

$$\xi_i, \xi_i^* \geq 0$$

Here, $\phi(x_i)$ is the feature mapping induced by the kernel function, ϵ defines the margin, and ξ_i and ξ_i^* are slack variables.

The slack variables that allow for deviations from the ϵ-tube. C is the regularization parameter. It controls the trade-off between achieving a low error on the training data and ensuring that the model generalizes well to unseen data. SVR uses a margin of tolerance (ε) where deviations within this range are ignored. SVR tries to fit the best regression line within this margin, keeping the errors as small as possible. SVR can work with linear and non-linear data by applying a kernel function (e.g., linear, polynomial, radial basis function - RBF). The kernel trick transforms the original data into a higher-dimensional space where a linear regression model might better fit the data.

2.3.3 K-Nearest Neighbour Regression

K-Nearest Neighbour (KNN) Regression [14] makes predictions based on the local relationships between data points. It predicts the value of a target by considering the k-nearest neighbors in the training data (based on features) and averaging their target

values. For set of features X={x_1, x_2,. . . , x_n} and target values Y={y_1, y_2,…y_n}, the KNN regression prediction is given by,

$$y' = 1/k \sum_{i \in k(x)} yi$$

where, k(x) is the set of k-nearest neighbors of the input point xi, and yi is the target value of the i-th neighbour.

2.3.4 Decision Tree Regression

Decision Tree Regression [16] works by building a tree. A decision tree is composed of internal nodes and terminal nodes (leaves). Each internal node represents a decision based on a feature, and each branch represents the outcome of that decision. The leaves contain the predicted target value. The dataset is recursively split into two branches at each node. The goal is to minimize the difference between the actual target values and the predicted target values by selecting the optimal split point at each node. The most common splitting criterion is to minimize the Mean Squared Error (MSE). The splitting continues until a specific stopping condition is met, such as reaching a maximum depth or minimum number of samples in a node.

2.5.5 Bagging Regression

Bagging Regression [18] is Bootstrap Aggregating, which is an ensemble learning technique designed to improve the accuracy and stability of machine learning algorithms, particularly those prone to high variance, such as decision trees. Bagging works by training multiple decision trees on different random subsets of the training data and then averaging their predictions for regression tasks.

2.5.6 Random Forest

Random Forest Regression [17] is an ensemble learning method used for regression tasks. It operates by constructing a multitude of decision trees during training and outputting the average prediction of the individual trees for regression tasks. This method enhances the predictive accuracy and controls overfitting by combining the predictions of multiple models.

Random Forest initially creates multiple datasets by bootstrapping. Specifically, bagging is used, where sampling is done by replacement to create different subsets of the

original dataset. For each bootstrapped dataset, a decision tree is built. At each split in the tree, a random subset of features is chosen, and the best split from this subset is used. Once the forest of trees is built, predictions are made by averaging the predictions from each tree (for regression). By averaging the results of many decision trees, Random Forest reduces the risk of overfitting that is common in individual decision trees. Unlike bagging regression, where each decision tree uses all the features available in the dataset; Random Forests introduce another layer of randomness by selecting a random subset of features at each split of the decision tree. This reduces correlation between the trees and further improves generalization.

2.5.7 Gradient Boosting Regression

Gradient Boosting Regression [19] is also an ensemble method that creates ensemble of decision trees in a sequential manner. Each successive model tries to correct the errors of the previous models by minimizing a loss function using gradient descent. Unlike Random Forest, where trees are trained independently, Gradient Boosting trains trees sequentially. Each new tree is trained to correct the residuals (errors) of the previous trees.

2.5.8 Ada Boost Regression

AdaBoost [20] is also an ensemble method that works by combining multiple weak learners into a single strong learner. It adjusts the weights of data points that are hard to predict. AdaBoost focuses on improving the performance of the weak learners by emphasizing the data points where the model performs poorly. Unlike Gradient Boosting, AdaBoost modifies the weights of the samples based on the absolute errors in regression tasks. Samples with larger errors will be given more weight, encouraging the next learner to focus on these difficult-to-predict points.

2.4 Model Selection

ANNs are highly flexible and can model complex relationships in the data. However, they generally require large amounts of data to train effectively, which is generally not there in alloy design. Thereby, use of ML algorithms can offer better results if there is less data. Genetic algorithms (GA) are optimization approaches based on natural selection. They perform effectively in circumstances where the search space is

huge and unexplored, as is frequently the case in alloy design. Another advantage of the GA approach is its high level of customization. Prerequisites can be easily imposed to exclude unwanted candidates throughout the selection process. From the above discussion, this study proposes to use ML in conjunction with GA optimization, for single-objective alloy design task. This work proposes using machine learning algorithms (Linear Regression, SVR, KNN- Regression, Decision Tree Regression, Bagging Regression, Random Forest, Gradient Boosting and Ada Boost Regression) in conjunction with GA optimization for a single-objective alloy design assignment. The limitation of GAs is that they are computationally expensive. Since the target is of more accurate model, computationally intensive technique is acceptable.

2.5 Evaluation metrics for ML models

2.5.1 Mean Absolute Percentage Error (MAPE)

MAPE is a measure of prediction accuracy in a regression model, expressed as a percentage. It is calculated as the average absolute percentage error between the predicted and actual values. It is given by the formula,

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{y_i - y_i'}{y_i} * 100$$

2.5.2 R^2 Evaluation

The R^2 evaluation parameter is a statistical measure that represents the proportion of the variance in the dependent (target) variable that is predictable from the independent (feature) variables. The R^2 is calculated using the following formula:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - y_i')^2}{\sum_{i=1}^{n}(y_i - Y)^2}$$

Where, y_i is the value of target variable, y_i' is the predicted value of the target variable, Y is the mean of the actual target variable and n is the number of data points. Higher values of R^2 indicate a better fit of the model to the data, meaning more of the variance is explained by the features. $R^2 = 1$ is a Perfect fit model and the model explains 100% of the variance in the target variable. If for a model $R^2 = 0$, then the model does not explain any of the variance; it performs no better than simply using the mean of the

target variable. For models with $R^2 < 0$, the model performs worse than the mean model, which means that the predictions are off by more than if you had just predicted the mean for every data point.

Chapter 3

METHODOLOGY

3.1 Alloy design for target mechanical property

The machine learning algorithms are capable of predicting the target based on the feature values. The dataset comprises of alloy compositions using different elements as the features and a single mechanical property as the target variable. Let *X* and *y* denote the features and target for the machine learning model. Where, $X \in \mathbb{R}^{nxp}$ represent the element composition matrix, for *n* is training samples, and *p* elements. $y \in \mathbb{R}^{n}$ represent the target value of a specific mechanical property. The training of a model $M(X, \theta)$ involves finding the optimal parameters θ that minimize the loss function *L* over the entire training dataset. Where the loss function $L(y, M(X, \theta))$ indicates the error between the predicted values $M(X, \theta)$ and the true output value *y*. This can be formulated as follows,

$$\theta^* = argmin_\theta \frac{1}{n} \sum_{i=1}^{n} L(y_i, M(i, \theta))$$

In the above equation θ^* is the set of optimal parameters.

However, the objective of the work presented is to find the composition of the alloy elements for a desired target mechanical property, which is an inverse design problem. The inverse design cannot be addressed by simply considering a mechanical property as feature and multiple target values (composition values of elements), as the model may not perform well. Thereby, the inverse problem is addressed as an optimization problem by use of genetic algorithm. An overview of the proposed method for predicting alloy composition considering a single desired value of UTS or EC is presented in figure 3.1.

First, experimentation is performed using various regression models. The best model is selected depending on the results in order to obtain important features for the final model development. The forward regressor is built using the selected features and

the selected model. Along with the selected model an inverse model is also trained along with application of genetic algorithm. The results of this inverse model is validated using the forward regressor, as the forward models have better performance due to availability of more features. Various modules of the proposed method are discussed next.

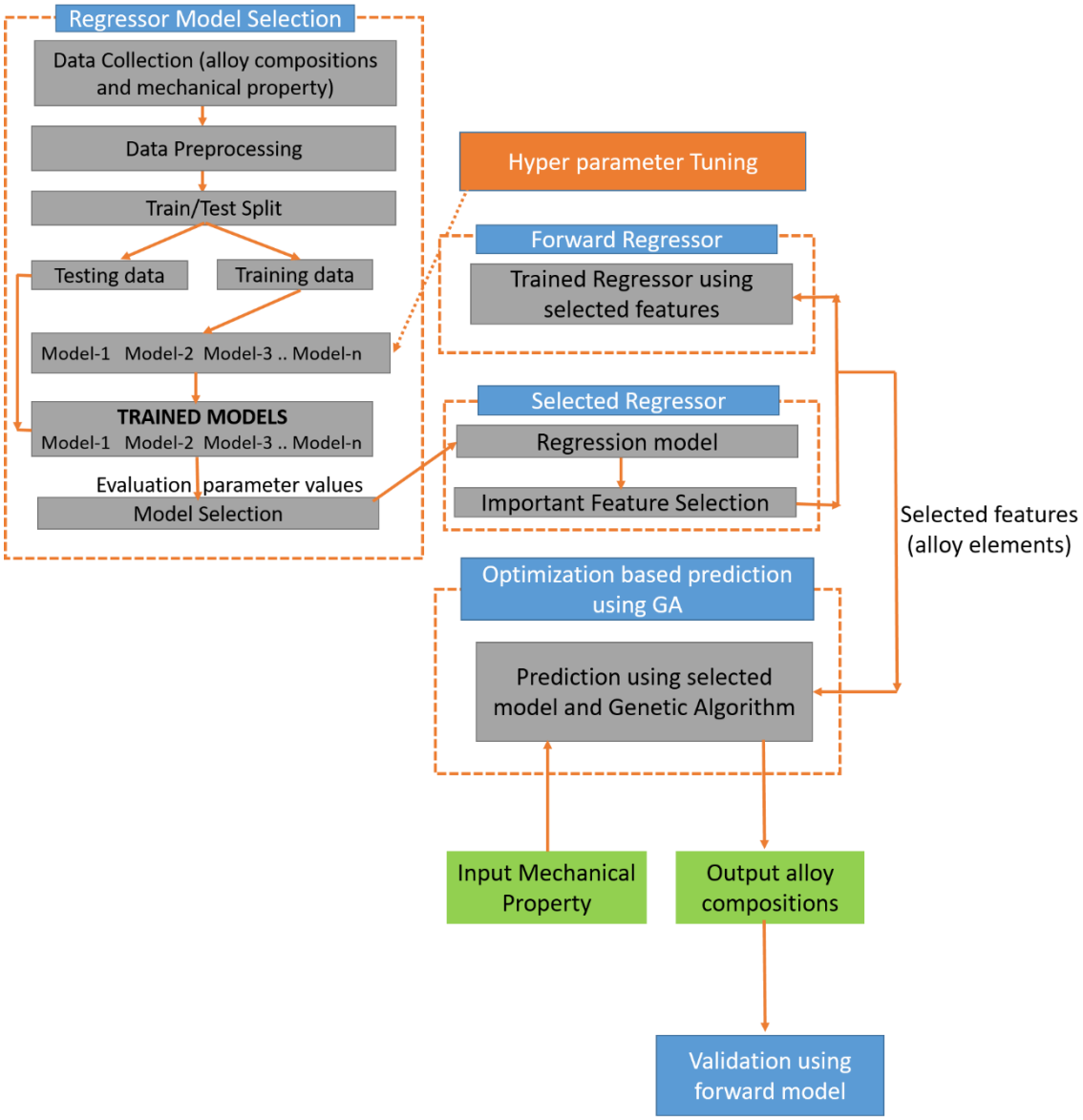


Figure 3.1: Proposed method for alloy design for single target property value

3.1.1 Regressor Model Selection

Various machine learning models, namely, Linear Regression, SVR, K-NN Regression, Bagging Regression, Decision Tree Regression, Random Forest Regression,

Gradient Boosting Regression and AdaBoost Regression, are trained using the training set. All these models are trained using composition elements as the features and mechanical property value as the target. The best performing model based on the R^2 value is selected as Regression Model. For all the models hyper-parameter tuning is performed. It is a crucial step in optimizing ML models. Hyper-parameters are the configuration settings that are not learned from the data but are set before the training process begins. Each ML algorithm has its own set of hyper-parameter. For example, number of estimators, maximum depth of each tree, minimum samples to split a node, minimum samples per leaf, number of features for splitting, bootstrap, etc.

3.1.2 Selected Regression Model and Forward Design

Selecting the most important features for training the model is a crucial step in machine learning. Irrelevant features may reduce the models predictive accuracy. Too many features can cause the model to t to noise rather than the underlying data patterns, leading to overfitting. Use of only important features can remove noise, reduce overfitting and can help the model generalize better to new data. Thereby, we use only the important features (I) for building the forward regressor, where $I \in p$. The most important features are found using the selected model. The forward regressor is used to validate the output generated by the inverse model.

3.1.3 Optimization for prediction using Genetic Algorithm

An inverse model in machine learning refers to the task of estimating or predicting the input features that would produce a given target output from a model. This is the reverse of the typical task where the input features are used to predict the target output. This can be expressed as:

$$X = M^{-1}(X, \theta)$$

where, X is the input and y is the target.

However, all models may not have a straightforward inverse. For linear models, an inverse exists, but for complex nonlinear models, finding the inverse may be more difficult or may not be uniquely defined. This can be addressed as optimization problem to find the X that minimizes the error between the output of the model and the given target y, by application of genetic algorithms.

Algorithm 1 Optimization using Gradient Boosting and Genetic Algorithm

INPUT:

- Trained Gradient Boosting Regressor GBR mapping from feature space (compositions) $x \in \mathbb{R}^m$ to target space of mechanical property $\hat{y} \in \mathbb{R}$.
- Desired target value of mechanical property $y_{target} \in \mathbb{R}$

OUTPUT: A feature vector $x^* \in \mathbb{R}^m$ such that $GBR(x^*)$ is as close as possible to y_{target}.

Step 1: Initialize the Population $\mathcal{P}_0$
Initialize population $\mathcal{P}_0 = \{x_1^0, x_2^0, \cdots, x_N^0\}$
This is considerd as generation at t=0

Step 2: Evaluate Fitness
For each feature vector $x_i^t \in \mathcal{P}_t$, evaluate the fitness function $F(x_i^t)$ as,
$\hat{y}_i^t = GBR(x_i^t)$
The fitness function is computed using mean squared error (MSE) between the predicted and actual target values,
$F(x_i^t) = -|y_{target} - \hat{y}_i^t|$

Step 3: Selection
Select individuals for reproduction based on fitness $F(x_i^t)$

Step 4: Crossover
Perform crossover between selected pairs (x_A^t and x_B^t) to generate offspring.
Single point crossover is done. Elements of feature vector are swapped based on a crossover point c.

$$x_{offspring} = \begin{cases} x_A^t[i] \text{ for } i \leq c \\ x_B^t[i] \text{ for } i > c \end{cases}$$

Step 5: Mutation
Apply mutation with probability $\mathcal{M}$ to introduce variations to the offspring vectors by adding Gaussian noise.

Step 6: Replacement
Replace $\mathcal{P}_t$ with new population $\mathcal{P}_{t+1}$

TERMINATION: Repeat steps 2 to 6 for a fixed number of generations G

A genetic algorithm (GA) is an optimisation method that draws inspiration from biology's genetics and natural selection processes. It makes use of random searches combined with previous data to lead the search to the region of best performance in the solution space. It is widely utilised to produce high-quality solutions for optimisation and search problems. Algorithm 1 presents how Gradient boosting and Genetic Algorithm are used for prediction of best alloy compositions using optimization. The algorithm considers the trained GRB model and provides a target value for the desired mechanical property and predicts the value of each component. In step 1, the population (value of each feature) initialization is done randomly. However, we specify the minimum and

maximum value for initialization of the population, leading to a better initialization and composition values. The candidate solution is passed to step 2. In this step fitness value is computed using Mean Squared Error (MSE) function. Using these step 3 selects the individuals for reproduction. Step 4 performs crossover to generate new o spring. These are slightly altered in step 5 to introduce diversity. Using the current population and new offsprings, updated population for the next generation is output in step 6. These steps are repeated for 100 generations.

3.1.4 Verification

To verify if the output values *X'* from the optimization model will give correct *y* value, the value of *X'* is given as input to the forward regressor. If the value obtained *y* from the forward regressor and *y*' are same or close then we can conclude that the inverse design (uisng GBR and GA optimization) is giving the correct composition for the target mechanical property.

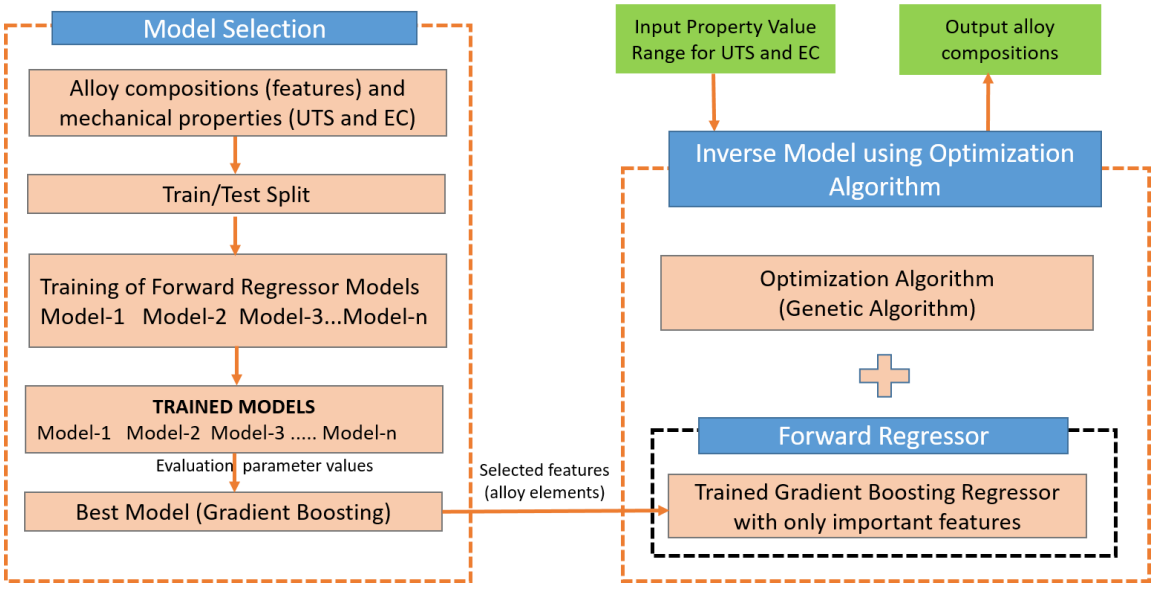

Model Selection
Alloy compositions (features) and mechanical properties (UTS and EC)
Train/Test Split
Training of Forward Regressor Models
Model-1 Model-2 Model-3...Model-n
TRAINED MODELS
Model-1 Model-2 Model-3 ..... Model-n
Evaluation parameter values
Best Model (Gradient Boosting)
Selected features (alloy elements)
Input Property Value Range for UTS and EC
Output alloy compositions
Inverse Model using Optimization Algorithm
Optimization Algorithm (Genetic Algorithm)
Forward Regressor
Trained Gradient Boosting Regressor with only important features

Figure 3.2: Proposed method for multi-objective alloy design

3.2 Multi-objective Alloy design for Simultaneous Enhancement of UTS and EC

The same method (as discussed in Section 3.1) is used for simultaneous enhancement of UTS and EC. The overview of this method is presented as figure 3.2. As discussed,

GBR performs the best individually for UTS and EC. From these models, the most important features (alloy elements) are selected. For example, if I_{UTS} are important features for UTS model and I_{EC} are important features for EC model then, important features used to train the forward regressor are $I_{UTS} \cup I_{EC.}$ Let these models be m^*_{uts} and m^*_{ec}. These are used in conjunction with optimization algorithm to maximize both UTS and EC.

The aim is to find the composition values $X=\{x_1, x_2, \ldots x_j\}$ that maximize target values of y_1 and y_2, where y_1 is UTS and y_2 is EC. For this Genetic optimization algorithm is used that predicts the element composition, such that the obtained values of X minimize model errors for both m^*_{uts} and m^*_{ec}.

The target values to be attained for both UTS and EC are specified in range. The target values of 500-900 is set for UTS and 40-90 is set for EC. For each alloy composition that is predicted by the optimization algorithm, the forward regressor is used to compute the UTS and EC value. The Mean Squared error was computed for each and a penalty score was found out. This penalty value acts as a feedback to the optimization algorithm and adjusts the prediction.

Chapter 4

RESULTS AND DISCUSSION

4.1 Dataset

The chemical composition and mechanical properties data of different alloys from published literature was collected [16]. The alloy data of all series are included for making a model in the present work. There are 12 elements forming the composition namely, Al, Si, Fe, Cu, Mn, Mg, Cr, Ni, Zn, Ga, V, and Ti. The value of Al is computed as balance based on the weight percentage of other elements. A snapshot of the dataset is presented in Table 4.1. The mechanical properties of Ultimate Tensile Strength (UTS) and Electrical Conductivity (EC) values are recorded for each composition. The dataset comprises of composition data for 176 alloys for UTS. Different temper types are also considered. There are a total of 103 instances in the dataset for EC. UTS is measured in MPa, and EC is measured in %IACS (International Annealed Copper Sttandard) at 20℃.

Table 4.1: Dataset Screenshot.

Alloy number	Al	Si	Fe	Cu	Mn	Mg	Cr	Ni	Zn	Ga	V	Ti	UTS
1060	99.60	0.25	0.35	0.05	0.03	0.03	0	0	0.05	0	0.05	0.03	85
1100	99.00	0.15	0.38	0.125	0.05	0	0	0	0.10	0	0	0	110

4.2 Correlation Analysis

To understand the relationship between elemental composition and mechanical properties, correlation analysis is performed on the self-created dataset. The statistical correlations between different elements and mechanical properties are investigated using Spearman correlation. Since the Spearman Coefficient takes into account any monotonic relationship, while the Pearson Coefficient only takes into account linear correlations, Spearman correlation is employed [36]. As a result, non-linear relationships between two variables are accurately represented. It is also less susceptible to outliers.

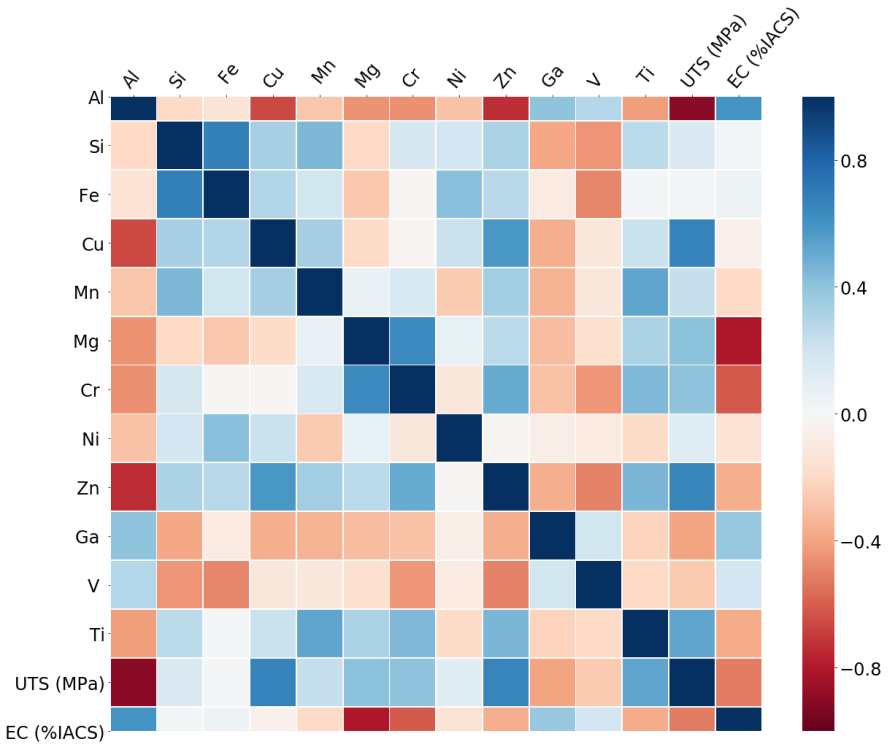


Figure 4.1: The heatmap of statistical correlation among compositions and properties UTS and EC. The bar shows the color scheme representing the different values of Spearman's rank correlation coefficients.

The correlation matrix is presented in figure 4.1. Various insights that can be inferred are:

- Cu, Mg, and Zn show positive correlation with UTS. UTS is the maximum stress that a material can withstand while being stretched or pulled before breaking. Copper increases strength through solid-solution strengthening and precipitation hardening. In particular, copper atoms distort the metal lattice and hinder the movement of dislocations, which increases UTS. Zinc is a primary alloying element in brass, which is known for its excellent strength and corrosion resistance. Zinc also contributes to the high strength-to-weight ratio in aluminum-zinc alloys (e.g., 7xxx series of aluminum alloys) used in high-performance applications like aircraft structures. This is why alloys containing Cu and Zn are extensively used in applications where both high tensile strength and yield strength are crucial, such as aerospace, automotive, and structural engineering.

- Elements Cu, Mn, Mg, Cr, Zn and Ti have strong negative correlation with EC. Electrical Conductivity refers to a material's ability to conduct electricity. A negative correlation with elements like Cu, Mn, Mg, Cr, Zn, and Ti suggests that adding more of these elements into an alloy or material will reduce the material's ability to conduct heat and electricity. Copper (Cu) is known for its high electrical conductivity, but when alloyed with other elements like Mn, Mg, Cr, Zn, and Ti, the conductivity decreases. For example, brass (Cu-Zn alloy) has lower conductivity compared to pure copper.
- UTS and EC shows strong negative correlation, which indicates that increase in UTS reduces EC and vice versa. Thereby, simultaneous enhancement of these properties is a challenge.

4.3 Performance of individual ML models for UTS and EC

4.3.1 Experimentation and Results on self-created dataset

In this section the results of various ML models are discussed. Eight ML models are trained using 12 element compositions for each UTS and EC as the target feature. The model performance results are presented in Table 4.2 and a visual representation of R^2 values of Gradient boosting algorithm is shown in figure 4.2. As observed, GBR gives the best results for UTS as well as EC. Therefore, GBR is selected as the regressor model. Important features that most impact UTS and EC are then found. GBR inherently calculates feature importance during the training process. It evaluates how much each feature contributes to reducing the error at each split of the decision trees. The feature importance values are directly extracted from the trained model using "feature_importances_" parameter of the trained model using sklearn library in python. The important features are shown in figure 4.3. Based on this Al, Si, Fe, Cu, Mn, Mg, Cr, Zn and V are selected as the features for training the simultaneous model.

Table 4.2: Performance of individual models trained for UTS and EC as target feature.

Method	UTS		EC	
	MAPE	R^2	MAPE	R^2
Linear Regression	12.95	0.85	18.71	0.11
SVR	14.43	0.88	13.88	0.58
KNN regression	13.18	0.87	8.34	0.80
Decision Tree Regression	14.95	0.83	8.57	0.70
Random Forest	16.76	0.80	9.28	0.72
Bagging Regression	13.38	0.86	8.84	0.77
Gradient Boosting Regression	**8.93**	**0.91**	**7.35**	**0.86**
Ada Boost Regression	14.80	0.88	8.53	0.79

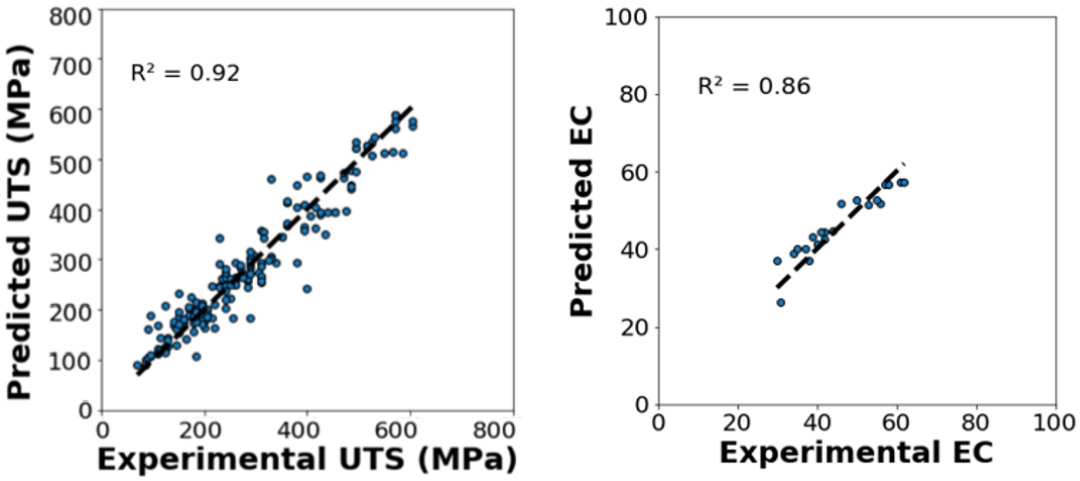


Figure 4.2: R^2 for UTS, and EC using Gradient Boosting for predicted and experimental values.

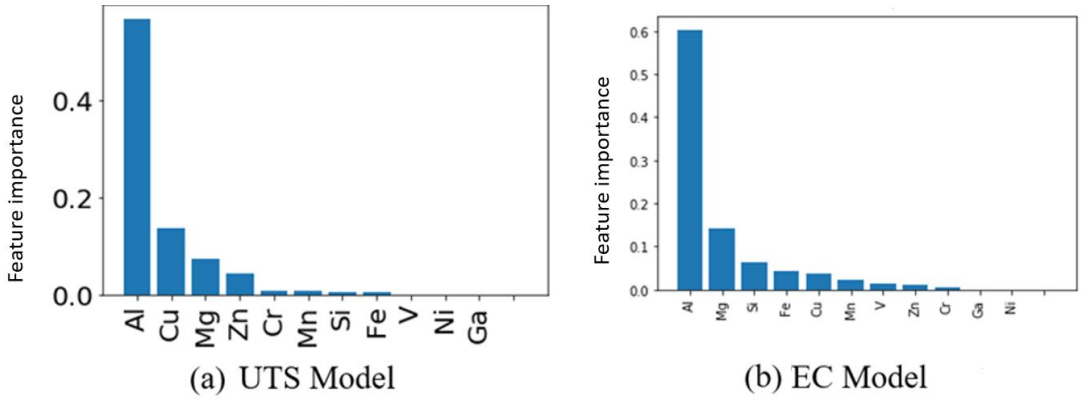


Figure 4.3: Important features (a) UTS (b) EC.

4.3.2 Obtained Alloy Compositions

The experimental values of various compositions for input mechanical properties are presented in Table 4.2 and 4.3. When an input mechanical value is provided the optimization model provides alloy composition and its mechanical value computed by GA. This is also validated with the forward regressor (gradient boosting) as presented in the last column of the tables. As observed in the composition values produced by the ML models, table 4.3 shows that elements Cu, Mg, Cr and Zn have impact on UTS. Higher composition of Cu is observed in EC compared to other elements in Table 4.4.

Table 4.3: Predicted alloy composition for different UTS values.

Target UTS Value	Alloy composition (wt%)								UTS using proposed method (in MPa)	Predicted value using forward GBR (in MPa)
	Al	Si	Fe	Cu	Mn	Mg	Cr	Zn		
400	76.25	1.46	3.07	4.12	0.22	4.40	5.39	5.06	408.5	410.2
500	77.12	0.46	1.73	2.00	0.37	3.45	6.99	7.84	499.9	499.9
560	81.16	0.10	0.10	4.62	0.64	3.93	3.17	6.26	570.0	566.3
650	86.72	0.00	0.00	2.66	0.00	2.60	2.00	6.00	620.0	615.0

Table 4.4: Predicted alloy composition for different EC values.

Target EC Value	Alloy composition (wt%)									EC using proposed method (%IACS)	Predicted value using forward GBR (%IACS)
	Al	Si	Fe	Cu	Mn	Mg	Cr	Zn	V		
30	87.03	0.09	0.58	9.18	1.00	1.00	1.00	0.00	0.10	30.0	33.0
40	90.58	0.00	1.00	5.16	1.00	0.54	0.71	1.00	0.00	40.0	40.5
50	91.30	0.00	1.00	5.22	0.59	0.00	1.00	0.87	0.00	50.9	51.4
60	95.43	0.57	0.66	1.20	0.00	0.53	0.58	1.00	0.00	60.0	59.9

4.3.3 Experimentation and Results on Existing Data

To further validate if the models can generalize well, experiment on existing data [37] is also performed. There are 25 element compositions in the dataset Al, Ag, B, Be, Bi, Cd, Co, Cr, Cu, Er, Eu, Fe, Ga, Li, Mg, Mn, Ni, Pb, Sc, Si, Sn, Ti, V, Zn, Zr and 1121 rows in total. The mechanical properties available are Elongation, Tensile Strength, and Yield Strength. The important features found for Tensile Strength property are Al, Cu, Fe, Li, Mg, Mn, Sc, Si, Zn, Zr as shown in figure 4.4. The obtained results are

presented in Table 4.5. It is observed that the results obtained using a much smaller dataset that we created as compared to this dataset are also consistent with the results obtained using this dataset.

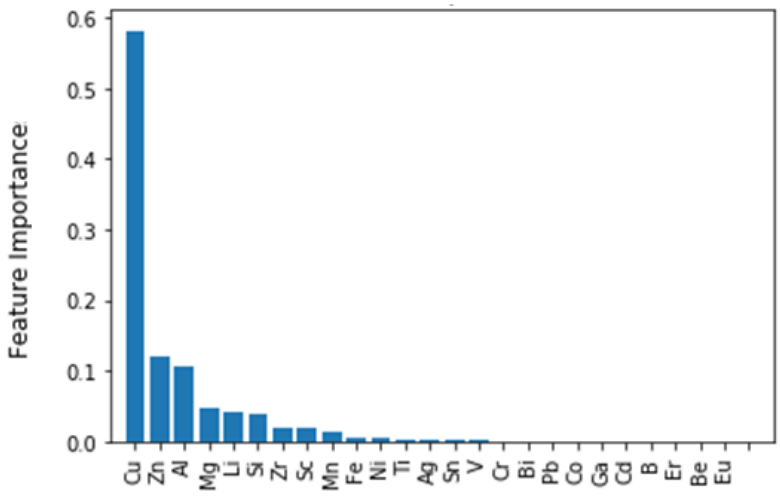


Figure 4.4: Selected features for Tensile Strength model

Table 4.5: Composition for different UTS values using optimization algorithm for existing dataset.

Desired UTS Value	Alloy composition (wt%)										UTS using proposed method (in MPa)	Predicted value using forward GBR (in MPa)
	Al	Cu	Fe	Li	Mg	Mn	Sc	Si	Zn	Zr		
300	84.61	0.00	2.12	4.93	5.00	5.00	4.43	4.72	0.00	1.46	292.4	305.0
400	82.41	5.00	0.80	0.00	0.00	1.91	0.00	0.00	0.33	4.79	406.9	385.2
500	76.21	1.07	0.46	4.71	0.00	0.85	2.84	0.00	3.61	4.49	503.6	502.6
550	83.34	2.55	1.92	2.72	4.61	4.66	4.24	2.81	2.37	4.11	552.0	530.3
600	80.14	3.68	0.00	3.85	1.06	0.00	0.00	4.70	0.74	2.68	603.1	595.0
650	76.65	4.90	0.00	0.00	0.92	0.00	1.66	3.13	0.62	3.38	650.0	618.0
700	70.68	2.06	0.00	0.00	3.16	3.68	0.09	1.72	0.70	4.29	685.0	699.0

4.3.4 Testing on data from literature

To further assess the model, Al alloys presented in the literature are used to find the target properties. Since, these are not used in model training, it provides an unbiased evaluation of the models and reflect the generalization ability of tuned models. The test results are presented in Table 4.6. The testing is performed using the forward regressor. It is observed that most of the predicted values are close to those reported in the

reference paper. Although, these values are close, it is observed that the predicted values are less than those reported. This can be attributed to physical experimentation values being reported in these papers with various post processing steps being applied to increase the property values, like solution treatment in [38].

Table 4.6: Property Prediction for Alloy Composition

Ref	Alloy composition (wt%)											Target UTS values as reported (in MPa)	Target UTS values predicted by our model (in MPa)
	Al	Zn	Mg	Cu	Mn	Fe	Si	Cr	Zr	Ti	Sc		
[38]	87.35	1.86	2.21	0.94	1.68	3.85	2.11	0.00	0.00	0.00	0.00	581	542
[39]	86.65	8.90	2.29	1.76	0.10	0.00	0.00	0.14	0.10	0.06	0.00	700-750	712.6
[40]	89.12	5.87	2.07	2.42	0.11	0.10	0.16	0.00	0.10	0.05	0.00	577	560
[41]	87.61	7.81	1.93	2.24	0.00	0.00	0.00	0.00	0.16	0.00	0.25	628-679	601

4.4 Performance of Multi-objective Model for Simultaneous enhancement of UTS and EC

4.4.1 Experimentation and Results

In this section the results obtained for alloy prediction using Gradient Boosting with various optimization algorithms for multi-objective UTS and EC model are reported. Table 4.7 presents the compositions using Bayesian optimizer, table 4.8 shows compositions obtained using GBR and Simulated Annealing optimizer. Table 4.9 and 4.10 present the results for Particle Swam and Genetic Algorithm respectively.

Table 4.7: Alloy composition using Gradient Boosting with Bayesian Optimization.

Result No.	Al	Si	Fe	Cu	Mn	Mg	Cr	Zn	V	UTS	EC
1	95.60	0.81	0.87	0.73	0.41	0.23	0.36	0.36	0.59	416.4	34.7
2	87.66	0.69	0.71	4.00	0.92	2.00	0.72	3.00	0.27	577.3	31.5

Table 4.8: Alloy composition using Gradient Boosting with Simulated Annealing

Result No.	Al	Si	Fe	Cu	Mn	Mg	Cr	Zn	V	UTS	EC
1	84.94	0.57	0.74	7.47	1.47	3.89	0.26	0.49	0.11	477.8	34.2
2	86.91	0.47	0.96	1.03	1.72	3.10	0.26	5.52	0.00	505.4	33.4

Table 4.9: Alloy composition using Gradient Boosting with Particle Swam Optimization.

Result No.	Al	Si	Fe	Cu	Mn	Mg	Cr	Zn	V	UTS	EC
1	86.76	0.00	0.87	7.92	1.25	0.95	0.27	1.93	0.00	483.9	33.3
2	86.92	0.24	0.03	2.39	2.00	0.96	4.06	3.60	0.01	507.7	31.3

Table 4.10: Alloy composition using Gradient Boosting with Genetic Algorithm

Result No.	Al	Si	Fe	Cu	Mn	Mg	Cr	Zn	V	UTS	EC
1	**88.36**	**0.41**	**0.27**	**4.48**	**0.83**	**0.86**	**0.21**	**3.74**	**0.80**	**805.9**	**34.0**
2	81.05	0.97	0.90	5.84	1.55	3.67	0.27	5.32	0.39	790.2	34.0

The best values of UTS and EC are obtained using GBR with genetic algorithm. The best composition alloy is shown in Table 4.10 as Result no. 1. This proves the effectiveness of using GBR with genetic algorithm.

4.5 Experimental Validation by alloy casting

After obtaining the alloy compositions from proposed machine learning based model, a few samples were casted and tested for validating the tensile properties. The process for physical experimentation is given in figure 4.5. The cast alloy size for all the samples is shown in figure 4.6 (a). Figure 4.6 (b) shows a sample cast. The Cylindrical sample dimensions are presented in figure 4.7 and a few micro samples are shown in figure 4.8.

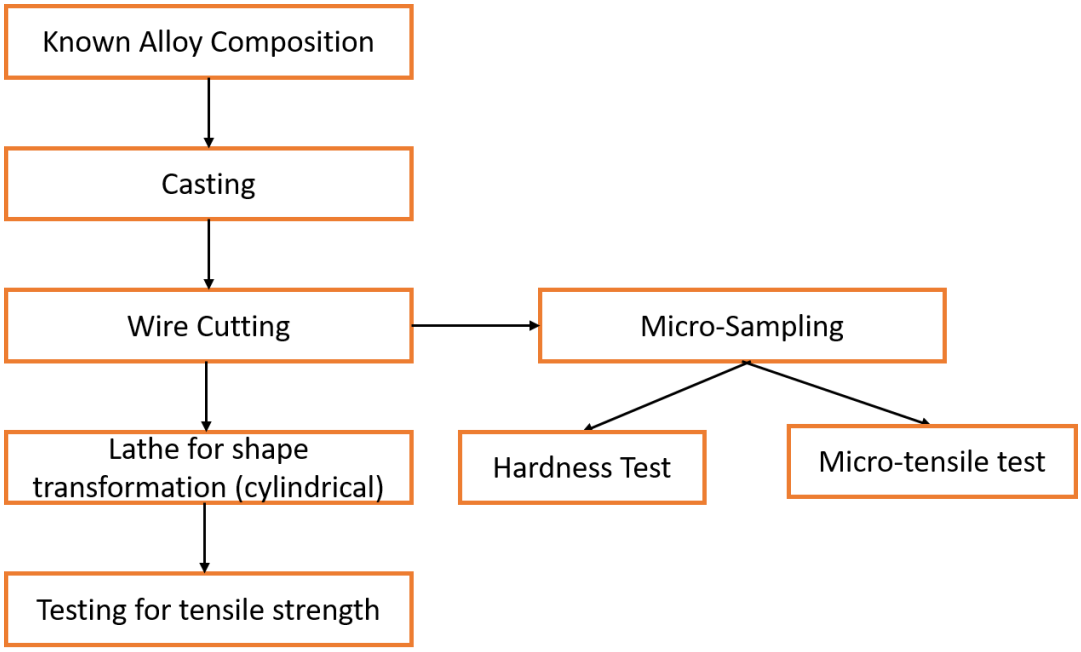
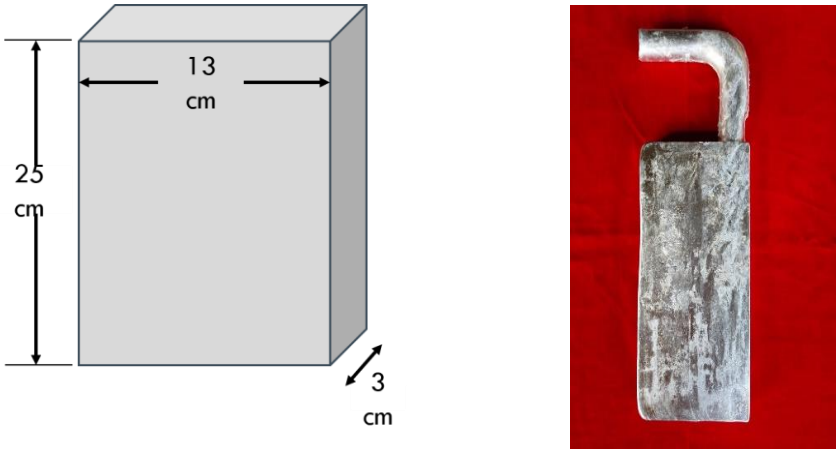


Figure 4.5: Process of physical sample validation for tensile strength.



(a) Cast Dimension **(b) Cast Sample**

Figure 4.6: Size of Al alloy cast block and Sample photo.

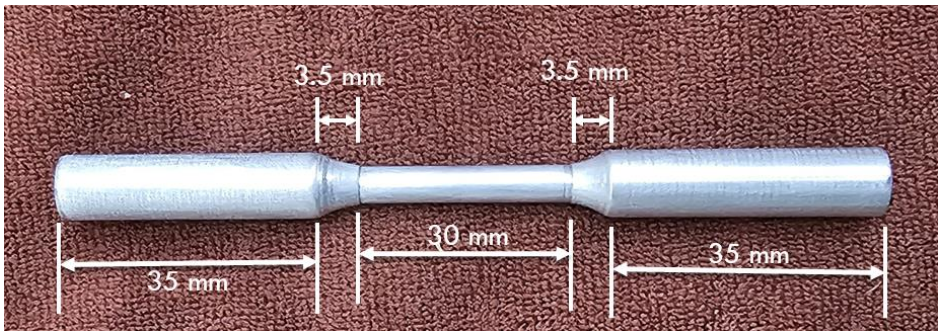
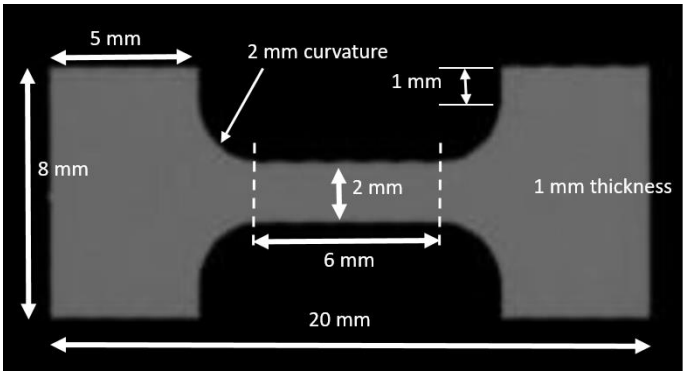


Figure 4.7: Sample Cylindrical Sample for Tensile Testing.



(a) Micro-sample Dimensions **(b) Micro-samples**

Figure 4.8: Micro-sampling samples.

4.5.1 Experimentation and Results on alloy composition for testing UTS

A. Al-Si Alloy

For experimental validation of the model, an Al-Si alloy with composition Al-10Si-0.35Mg was cast and thermo-mechanically processed to achieve a fine distribution of Si throughout the Al matrix. Tensile properties were measured for this alloy using universal tensile testing machine (Instron, UK). The elongation was measured with an extensometer. The stress-strain curve is shown in figure 4.9. The experimental UTS is 329.50 MPa. The predicted value of UTS by best model is 310 MPa. This suggests that the developed model is working perfectly. However, from metallurgical point of views, the UTS largely depends on the size distribution and the spacing of Si particles in the aluminum matrix. The distribution of Si for the above Al-Si alloy is shown in figure 4.10. The particle size is roughly 0.5 µm in size. Therefore, the UTS is very good in present case. The model which is developed uses best possible properties which can be obtained in the alloy system under consideration. Therefore, our validation is correct. The processing will differ from alloy to alloy and has to be considered while developing such models.

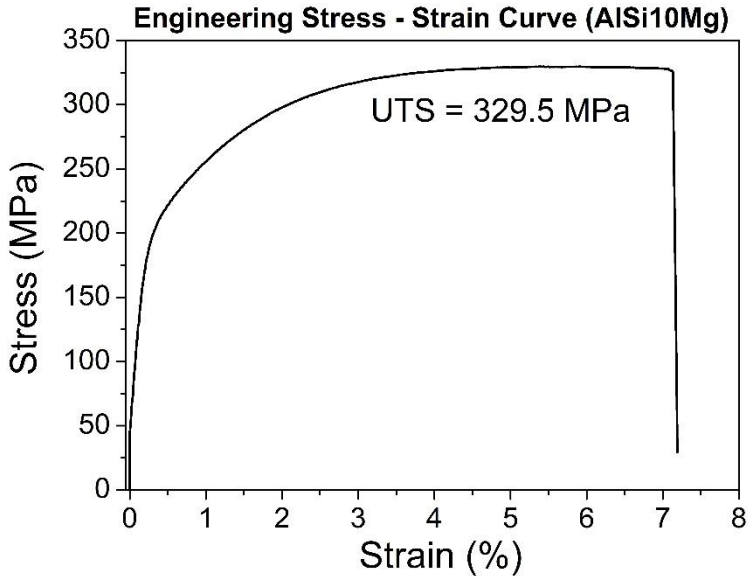


Figure 4.9: Stress-strain curve.

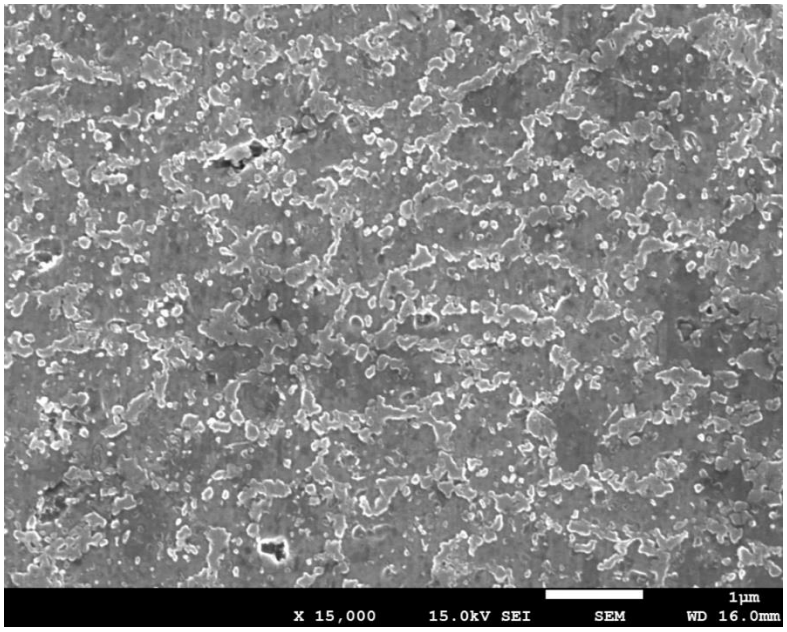


Figure 4.10: Distribution of Si in Al-Si alloy.

B. A643 Alloy

The alloy with best value for UTS from Table 4.3, Al-2.66Cu-2.60Mg-6Zn-2Cr (A643) was cast. This is the result obtained from individual model of UTS utilizing GBR and genetic algorithm. The alloy composition of the cast alloy was tested on Optical Emission Spectrometer (OES). OES is a powerful analytical instrument used for determining the elemental composition of metal alloys. It can identify which elements are present and in what concentrations, by analyzing the light emitted from a metal sample when it is excited by a high-energy source, usually an electric spark. The results of composition obtained are in Table 4.11. It shows that the composition is very close to the values provided.

The cylindrical sample as shown in figure 4.7 was built and tested. The UTS value obtained for A643 alloy of was found to be low as shown in Table 4.12, compared to the expected value. Although the value increase a bit by performing homogenization, still it was very low. The sample, therefore, was cut vertically to investigate the reason. It was found that there was lot of porosity in the alloy samples as shown in figure 4.11. Thereby, it was concluded that the sample was not fit for finding the tensile strength on UTM and micro-sampling was performed. The result of hardness test on micro-samples is presented in Table 4.13. The mean value of hardness was 159.8 HV with standard deviation of 11.9 HV. The tensile strength found was extrapolated (HV*3) and was found to be 480 MPa. Here was deviation and hence further investigation needs to be done on these samples. Also, the EC value obtained for the casted sample is 35.52.

Table 4.11: OES results for sample A643.

Element	ML based results given for casting	Results from OES
Al%	86.70	85.73
Fe	0	0.05
Si	0	0.05
Cu	2.66	2.99
Mn	0	0.001
Mg	2.60	2.50
Zn	6	6.52
Cr	2	2.05
V	0	0.009

Table 4.12: UTS Results for A643.

Sr. No.	Details	Temperature (Deg C)	Time (h)	UTS (MPa)
1	As-cast	-	-	118
2	Homogenization	500	8 + FC	148.9

Figure 4.11: Porosity in the cast materials. Visual observation with a normal camera.

Table 4.13: Hardness Results for A643 Aged condition.

Sample No.	Hardness		Sample No.	Hardness
1	171.2		8	174.3
2	136.8		9	160.6
3	176.9		10	157.9
4	155.2		11	163.3
5	163.3		12	176.9
6	142		13	145.8
7	151.6		14	163.8
Mean = 159.97 and Standard deviation=11.83				

Table 4.14: OES results for sample A646.

Element	ML based results given for casting	Results from OES
Al%	88.36	87.33
Fe	0.41	0.39
Si	0.27	0.48
Cu	4.48	5.10
Mn	0.83	0.75
Mg	0.86	0.64
Zn	3.74	3.87
Cr	0.21	0.22
V	0.80	1.13

4.5.2 Experimentation and Results on multi-objective alloy composition

Similar to testing on A643, the alloy composition from the multi-objective model having composition Al-0.41Fe-0.27Si-4.48Cu-0.3Mn-0.86Mg-3.74Zn-0.21Cr-0.80V (called as A646) is also performed. The results of OES are presented in Table 4.14 and were found to be close to the provided values. The UTS results are shown in Table 4.15. UTS of 290MPa was obtained on the sample that was subject to homogenization, solution heat treatment and aging. Further, hardening and tensile strength was tested on the micro-samples. These results are presented in Table 4.16. The mean value of hardness was 147.52 HV and Standard deviation is 7.96. For the sample, the tensile strength found is in the range of 406.5 to 467.74 MPa and EC is 23.96. The experimental values expected are 805.90 MPa for UTS and 34.07 for EC. Although the results are not very close to experimental results, but the suggested alloy is competitive with 2024 and some 6xxx and 7xxx alloys, which are commonly used in aerospace and structural applications. EC of 23.96 %IACS is moderate, but significantly higher than typical high-

strength 2xxx and 7xxx alloys, which often dip below 20%. The obtained result outperforms many existing aluminum alloys in terms of strength-to-conductivity balance, especially when compared to 2xxx and 6xxx series. It's a very promising result, for automotive light weighting with electrical functionality, or structural current-carrying components. The presence of Cu, Mg, and Zn suggests a design akin to 7xxx series, but the value of EC is better than most of them. Further, Cr and V additions likely improve grain refinement and precipitation strengthening. The manufacturing process needs to be optimized to produce near defect free alloys which can be aged to obtain peak hardness. The model results still remain promising, however processing results needs to be optimized.

Table 4.15: UTS Results for A646

Sr. No.	Details	Temperature (Deg C)	Time (h)	UTS (MPa)
1	As-cast	-	-	-
2	Homogenization (H)	500	8 + FC	166.4
3	Solution Heat Treatment (H+S)	500	2 + WQ	190.8
4	Aging (H+S+A)	175	8 + AC	290

Table 4.16: Hardness Results for A646 Aged condition

Sample No.	Hardness
1	155.8
2	141.9
3	135.5
4	150.6
5	146.0
6	155.3
Mean = 147.52 HV and Standard deviation=7.96	

Chapter 5

CONCLUSIONS

Creating new alloy compositions rapidly and enhancing existing alloys performance is the recent challenge in the field of metallurgical engineering. The work presented in this report, proposes a quick and efficient machine learning (ML) approach for alloy design. The following conclusions can be drawn:

- Alloy compositions can be designed quickly and efficiently by machine learning with proper hyper-parameter tuning. A forward and inverse model design were successfully implemented for Al alloy design. Gradient Boosting Regressor with Genetic algorithm as optimizer was found to be the best performing model.
- Al alloy for the best predicted target values were cast. The casted Al-10Si-0.35Mg alloy obtained UTS value of 329.5 MPa, which has model predicted value of 310 MPa. For A643, the mean value of hardness was found to be 159.8 HV, which was extrapolated (HV*3) to get the tensile strength as 480 MPa. The EC value obtained for the casted sample is 35.5 %IACS. For A646, the mean value of hardness was found to be 147.5 HV, gives UTS as 442.5 MPa, with EC as 23.9 %IACS. The results are suggestive that A643 with composition Al-2.66Cu-2.60Mg-6Zn-2Cr is a well-balanced alloy offering both high mechanical strength and relatively high electrical conductivity, which is rare in Al alloys. UTS value puts it on par with 7xxx series alloys, which are among the strongest Al alloys available and EC is significantly better than most high-strength alloys, which often fall below 25%.
- The results are indicative that machine learning can be leveraged for alloy design. Furthermore, incorporating additional training data or leveraging Generative AI techniques for synthetic data generation is expected to further enhance the experimental outcomes.

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